THREE-DIMENSIONAL DIGITAL MICROSTRUCTURE

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ABSTRACT

We report on a systematic means of generating a finite element (FE) mesh for realistic three-dimensional (3D) microstructure systems that are suitable for FE analysis. The relationship between a materials microstructure and its properties are well documented and drive efforts to model the substructure evolution of textured materials. An accurate 3D computer representation of the microstructure arrangement of a material is essential to modeling the behavior and performance of materials at the microstructure level. We describe a method that uses a combination of experimental and computational techniques to produce an accurate statistical representation of its microstructure arrangement. The experimental results are used to guide the construction of the abstract 3D digital model and to provide a quantitative measure for gauging the accuracy and quality of the model upon completion. Information about the size, shape, and orientation of the grains as well as the crystallographic orientation and miss-orientation between adjacent grains can be reproduced. A 3D advancing front grid-generating technique then uses this information to produce a tetrahedral volume mesh for the material that is suitable for FE analysis.

1. INTRODUCTION

The goal of the current work is to provide polycrystalline material modelers access to accurate three-dimensional (3D) digital microstructure models that are validated by direct comparison to experimental recrystallization data and an automated microstructure and grid-generation process to produce the finite element (FE) mesh for the complex microstructure systems. To accomplish this task, the results of two different efforts were modified and combined. One effort dealt with producing accurate 3D digital microstructure models and the other with generating the associated FE mesh for the microstructure system. The results of both of these efforts can be found elsewhere in the literature (Saylor, et al., 2004; Rollett, et al., 2004; Noack and Steinbrenner). This paper will focus on issues dealing with combining these two technologies and on the system to which they are applied. A brief overview of the two techniques will be provided to put this work into context with the overall objective.

2. TECHNICAL APPROACH

In recent years, significant progress has been made in modeling microstructure evolution during materials processing. These advances have been primarily in the area of application of continuum methods where empirical constitutive relations are used to describe the behavior of materials. These methods can be used to predict the final shape of a specimen following deformation processing and the temperature history of the material. However, these models have had little impact on the optimization of material properties because they cannot quantitatively determine, predict, or manipulate the internal structure of the material. Novel materials are often manufactured via advanced processing techniques that greatly influence the microstructure arrangement of the material and thus its properties. Manipulating the microstructure arrangement of materials is the primary mechanism that materials scientists and engineers have to optimize material properties. Material optimization through modeling and simulation will require researchers to develop new material models that link theories for the properties and performance of materials at the microstructure level with the thermo-mechanical processing steps required to produce them.

The process of taking materials from discovery to application can span years, even decades. Modeling and simulation is seen as a tool that can accelerate the process and minimize the cost of discovery,

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optimization, and insertion of these materials into new systems. Including microstructure description for materials at various levels is essential for developing realistic material models that have the predictive capability necessary for optimizing the performance and behavior of materials through modeling and simulation. The three critical elements of this technology are 1) an efficient process for generating the microstructure arrangement of a material that makes a quantitative connection between the experimental materials under study and the abstract 3D digital representation used in the simulations, 2) an efficient method for generating the FE mesh for the complex microstructure of the material at the grain level, and 3) physics-based material models that are accurate enough to predict the properties and performance of materials through modeling and simulations. Thus, the complex nature of modeling microstructure materials requires an automated microstructure model-building and discretization process of the grain structure prior to computational analyses. This paper will address the requirements needed for this type of material modeling technology.

2.1 Three-Dimensional Microstructure Geometry

In order to depict realistic processes giving rise to 3D microstructures, researchers at Carnegie Mellon University (CMU) developed a Microstructure Builder (MB) process that employs a combination of experimental and computational techniques to capture the complex microstructure arrangement of materials. This process is capable of producing accurate 3D digital microstructure model that is validated by direct comparison to experimental recrystallization data. In the initial step, a scanning electron microscope is used to examine the material under study and collect the data needed to characterize the microstructure arrangement of the material. Currently, data collected during the experimental stage is used to construct distribution functions for the size, shape, and orientation of the microstructure grains as well as the crystallographic orientation and miss-orientation between grains. The computational techniques of the MB then use the experimental distribution functions to guide the construction of the abstract 3D digital models. In the end, the characterization criterion provides a quantitative measure for gauging the accuracy and quality of the abstract model. This quantitative measure is used as the acceptance criteria in a Monte Carlo algorithm. The algorithm is capable of sorting through tens of thousands of possible microstructure configurations to gradually refine the model until the distribution functions converge. At this point, the two systems are considered statistically equivalent to the extent that the errors in the distribution functions are minimized. The results of the MB are then fed into the grid-generating algorithm to produce the FE mesh. The MB generates three files. The first file contains the coordinates for a set of points that are used to generate the Voronoi cells (Fig. 1). The second file contains information on how the Voronoi cells are combined to form the grains. Finally, the third file contains information on the crystallographic orientation of the grains.

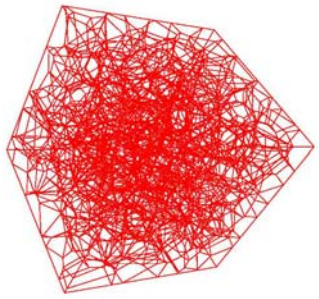

Fig. 1: Three-dimensional Voronoi tessellation representation of a single-phase microstructure.

2.2 Grid Generation

The process of meshing the microstructure system begins by decomposing the system into its various components (nodes, edges, faces, Voronoi cells [cells], and grains). Several preprocessing steps are needed to get the data in a form that can be used by the advancing front grid-generating algorithms, and several steps are needed to reassemble the results back into the original microstructure configuration. Below is a list of steps required to generate the FE mesh and to put the output into a format suitable for FE analysis for the digital microstructure generated by the MB:

1. The individual Voronoi cells are combined into grains.
2. Any faces connecting Voronoi cells of the same grain are removed.
3. Small edges are collapsed.
4. The edges are discretized.
5. The edges are recombined to the perimeter of the faces and used as input to the two-dimensional (2D) advancing front grid-generating algorithm.
6. The 2D advancing front grid-generating algorithm generates the surface mesh for the faces.
7. The faces are reassembled to form the surface of the grains and used as input to the 3D advancing front grid generating algorithm.
8. The 3D advancing front grid-generating algorithm generates the volume mesh for the grains.
9. The grains are reassembled and the connectivity is reestablished across the grain boundary.

10. The crystallographic orientation information is assigned to the elements of the FE mesh.
11. The results are output in a format that is suitable for FE analysis.

In the MB, grains are generated by combining one or more cells. In step one of the process, the cells used to construct each grain are identified and combined to produce the grains. Combining the cells to produce the grains has the undesirable effect of producing facets in the interior of the grains during the mesh-generating process. These facets are an artifact of the model-building process and could adversely affect the results of the simulations. In step two, we remove any interior faces of the grains.

Voronoi cells are perhaps not the best starting point for generating models for use in FE simulations. The process of generating Voronoi cells produces a large number of very small edges (compared to the desired element size). These small edges determine the size of the elements that will be produced during the meshing process. Elements that are too small will increase the computation time required for the simulation and can adversely affect the time step used in the FE simulation. In step three, edges that are below a certain threshold (input parameter) are collapsed to points. If the small edge belongs to a triangular face, the face is collapsed to an edge. This introduces some distortion into the model. Therefore, there is a limit to the size of the edges that can be collapsed.

In the next step, the remaining edges are discretized. This is an iterative process that starts by assigning a value for the maximum edge length to each node (node value). The node value is an input parameter that represents the desired element size. The length of all edges emanating from the nodes is then checked and if the current node value is larger than the smallest edge length, the node value is reset to the smallest edge length. The program then iterates over all of the edges and discretizes them, starting from the smaller of the two node values and proceeding to the larger. The calculations are made but the data is not stored during these iterations. The length of the segments grows geometrically until the larger node value is reached or the process terminates at the adjacent node. If the larger node value is reached, the remaining edge segments are equally spaced. If the larger node value is not reached before reaching the adjacent node, the node value of the adjacent node is reset to the value of the last edge segment length and a flag is set indicating that one of the node values was changed. The discretization continues until all of the edges have been split into segments. The code then checks the flag to see if any node values changed. The code continues the iterations until the process completes with out setting the node value flag. It then makes one last pass over the edges, performing the calculations and storing the discretization data.

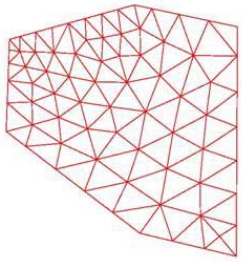

Fig. 2: Typical mesh generated by the two-dimensional advancing front grid-generating algorithm.

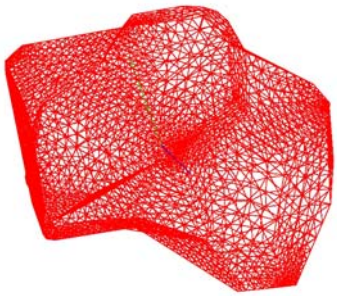

Fig. 3: The surface mesh for the grains is used as the starting point for the 3D advancing front grid-generating algorithm.

The edges are then reassembled to form the perimeters of the faces, and the edge segments are used as input to a 2D advancing front grid-generating algorithm to generate the FE mesh for the faces (Fig. 2). After all of the faces have been meshed, the faces are reassembled to form the surface of the grains (Fig. 3). This surface mesh is then used as input to a 3D advancing front grid-generating algorithm to mesh the grain volume. After all of the grains have been meshed, the grains are reassembled to form the original system with the FE mesh (Figure 4). During this process, all duplicate information is removed and the connectivity is established across the grain boundaries. The crystallographic orientation is assigned to the elements of the grains. Initially, all of the elements of an individual grain have the same orientation. In this way, grain boundaries arise naturally at the interface between adjacent grains due to the lattice mismatch between the grains and hence the differences in material properties. The spatial arrangement of the grains with different crystallographic orientation (texture) plays a key role in determining the properties of materials, and this simulation technique provides a tool for studying their relationship.

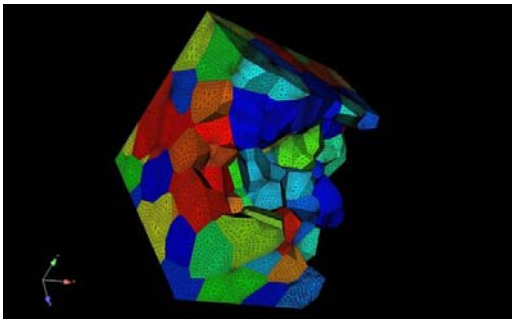

Fig. 4: Three-dimensional mesh for a sample of aluminum consisting of 134 grains.

CONCLUSIONS

These models provide researchers with an accurate geometric representation of the microstructure of single phase materials. However, to take full advantage of the models, computational methods that take advantage of the crystallographic information will need to be employed. One possibility is to integrate the crystallographic information into the constitutive equations and use crystallographic miss-orientation between adjacent grains to modify the grain-grain interactions. Fig. 5 shows how the crystallographic miss-orientation between adjacent grains produces an increase in strain at the grain boundaries in the simulation.

Another possibility is to replace common nodes along adjacent grain boundary faces with duplicate nodes (cohesive zones) to facilitate the simulation of sliding grain boundaries. Once again, the crystallographic miss-orientation between adjacent grains can be used to modify the material property of the cohesive zones between the grains. Fig. 6 illustrates the use of cohesive zones in simulating grain-grain interaction in a demo model generated by the MB. We are able to port the geometric models into ABACUS using cohesive zones. Current work is focused on automating the process for generating the cohesive zone models for larger simulations.

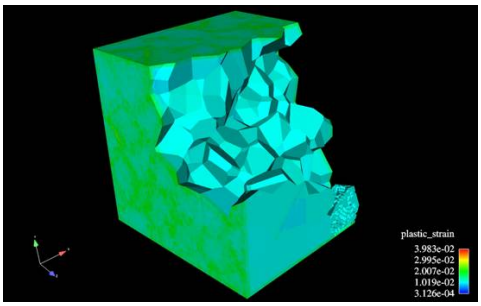

Fig. 5: The constitutive equations are modified to model the plastic strain as a result of the crystallographic miss-orientation between adjacent grains.

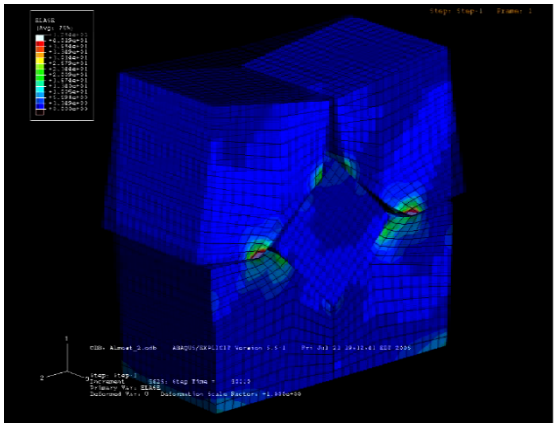

Fig. 6: Nodes between adjacent grains are duplicated and used to define the cohesive zones. The material properties of the cohesive zones define the interaction between the grains.

This is the first iteration of this software, and there are a number of improvements that can be made. Several steps in the mesh-generation process currently require input from the user that can be automated. In fact, once the data are collected from the electron microscope, the remaining process can be automated. Automating this process will significantly reduce the time required to set up simulations and give researchers access to realistic 3D digital microstructure models. It is our hope that the availability of these models will help stimulate research into the modeling and simulation of materials at the grain level.

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